

Remarks

Claims 1-13 and 16 are pending in the application. Claims 1 and 5 have been amended. Applicant respectfully requests entry of the foregoing amendments in order to place the application in better condition for allowance.

Applicants have filed herewith a Notice of Appeal. It is believed that no fee is due for the Notice of Appeal as the fee was previously paid on April 9, 2009.

Claim Rejections – 35 U.S.C. §112

Claims 1-13 and 16 have been rejected under 35 U.S.C. §112, second paragraph, as being indefinite for failing to particularly point out and distinctly claim the subject matter which applicant regards as the invention. The Examiner contends that in claim 1 it is unclear what the field is and further, that it is unclear with respect to the relationship between the field sample values and the field size values. Applicants have amended claim 1 to recite that the “field” is the electrostatic field. Claim 1 has been further amended to clarify that the field sample values pertain to the second molecule, and the field size values pertain to the first molecule.

The Examiner contends that claim 5 is unclear with respect to the term “absolute field size value”. Applicants have amended claim 5 as suggested by the Examiner to clarify that it is the “absolute value of the field size value” that is intended.

Claims 1-13 and 16 have been rejected under 35 U.S.C. §112, first paragraph, because the specification, while being enabling for electrostatic fields, does not reasonably provide enablement for any field. Applicants have amended claim 1 to recite that the field is an electrostatic field. In view of the amendment, Applicants respectfully request withdrawal of the rejection under 35 U.S.C. §112.

Claim Rejections – 35 U.S.C. §101

Claims 1-12 have been rejected under 35 U.S.C. §101 as being directed to non-statutory subject matter. The Examiner contends that in claims 1-12, no transformation is taking place.

Applicants respectfully disagree with the Examiner's contention. Claim 1 recites a computer-implemented method of identifying candidate molecules having a known biological activity or physicochemical property. The method includes the steps of providing a set of field points representing field extrema of a first molecule, wherein each field point has a position and a field size value, the molecule having a known biological activity or physicochemical property; determining at the position of each of the field points of the first molecule the field of a second molecule to obtain a set of field sample values; combining the field sample values with the field size values to provide a score indicative of the field similarity of the first molecule to the second molecule; and providing a measure of the second molecule to have the known biological activity or physicochemical property based on the score.

The claimed process satisfies the "transformation" prong of the "machine-or-transformation" test, and therefore is patent-eligible under §101. Under the transformation prong of the *Bilski* test, data transformations are acceptable if the data represents physical objects or substances (*In re Bilski*, 545 F.3d 943, 962-963, Fed. Cir. 2008). In the claimed process, the data that is transformed represents physical and tangible objects, and their respective structures. Specifically, the field points and field sample values represent information about particular molecules. As stated in the specification at page 4, lines 1-5:

The field point set encodes a large amount of information about the properties of the molecule, especially regarding its interaction with other molecules. The electrostatic field points encode information about the preferred hydrogen-bonding environment of the molecule, while the surface interaction field points encode the molecule's steric bulk.

As illustrated in Fig. 1, the molecular structure and interactions of formic acid are transformed into a set of field points. The field point data is further transformed to a score indicative of the field similarity of a first molecule to a second molecule. The score is used to identify the second molecule as a potential candidate molecule having a known biological or physicochemical activity. The transformation is central to the purpose of the claimed process. Moreover, the claimed process is not an abstract idea, but produces a tangible, real-world result in a form that is useful to the user of the

process. Specifically, the claimed process results in the identification of a molecule having a known biological activity or physicochemical property, which is useful to the user of the process in, for example, drug discovery and pharmaceutical research. Process claims 1-12 pass the "machine-or-transformation" test of *Bliski*, and are therefore drawn to patent-eligible subject matter. Applicants respectfully request the reconsideration and withdrawal of the rejection of claims 1-12 under 35 U.S.C. §101.

Conclusion

In view of the foregoing amendments and remarks, Applicants respectfully request entry of the forgoing amendment in order to place the application in better condition for appeal.

Respectfully submitted,

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/Sarah K. Varner /

June 3, 2010
Date